

# Effects of random fields on the dynamics of the one-dimensional quantum XXZ model

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## Abstract

The dynamics of the one-dimensional spin-1/2 quantum XXZ model with random fields is investigated by the recurrence relations method. When the fields satisfy the bimodal distribution, the system shows a crossover between a collective-mode behavior and a central-peak one with increasing field while the anisotropy parameter  $\Delta$  is small; a disordered behavior replaces the crossover as  $\Delta$  increases. For the cases of Gaussian and double-Gaussian distributions, when the standard deviation is small, the results are similar to that of the bimodal distribution; while the standard deviation is large enough, the system only shows a disordered behavior regardless of  $\Delta$ .

PACS numbers: 75.10Pq; 75.10.Jm; 75.40Gb; 75.50.Lk.

Keywords: Autocorrelation function; Spectral density; Quantum XXZ model; Random fields; Recurrence relations method.

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## 1. INTRODUCTION

Quantum spin systems are of considerable interest for the reasons that they provide a ground for studying quantum many-particle phenomena, and offer the possibility to compare the theoretical and experimental results, etc. The dynamical properties of the quantum spin systems have received much attention and a variety of achievements have been got over the years. Among the systems studied, the one-dimensional (1-D) spin-1/2 XXZ chain is one of the nontrivial models and has been used to describe several quasi-1-D compounds such as CsCoBr<sub>3</sub> [1–3], CsCoCl<sub>3</sub> [3, 4], Cs<sub>2</sub>CoCl<sub>4</sub> [5, 6] and TiCoCl<sub>3</sub> [7]. Concerning the dynamics of this model, the spin correlation function has been studied by using approximation and numerical methods [8–17]. Strong numerical evidence was found for a change of the bulk-spin autocorrelation function at  $T = \infty$  from Gaussian decay to exponential decay for the anisotropy parameter  $\Delta$  increasing from 0, and from exponential decay to power-law decay as  $\Delta$  approaches 1, then replaced by a more rapid decay upon further increase of  $\Delta$  [15]. The dynamics of the equivalent-neighbor XXZ model was studied in much detail at  $T = 0$  and  $T = \infty$  using different calculational techniques, and was found the same long-time asymptotic behavior for the correlation function [16, 17].

More efforts have been concentrated on the dynamics of random quantum spin systems in the past decades which can be used for describing more real materials such as ferroelectric crystals [18–21] and spin glasses [22]. Florencio and Barreto have studied the random transverse Ising model and obtained that the system undergoes a crossover between a collective-mode behavior and a central-peak one while the exchange couplings or external fields satisfy the bimodal distribution [23]. Later, the dynamics of the four-body transverse Ising model has been investigated for the cases of bond and field randomness [24], following which, a series of spin systems such as the XY model with zero magnetic, the transverse Ising model with Gaussian distribution and two-dimensional transverse Ising model etc. have also been studied [25–29]. A recent study shows that the next-nearest-neighbor interaction has a strong influence on the dynamics of the Ising system [30]. For the random XXZ model, the spin correlations have been investigated by using exact diagonalization [31], the real space renormalization group method [32–34] and a finite-chain study [35, 36] etc. Infinite temperature spin-spin correlation function has been found to display exponential localization in space indicating insulating behavior for large enough random fields [32]. The transverse

correlation function at  $T = 0$  has been found to exhibit a power-law decay to exponential decay depending on the exchange disorder [36].

In this paper, we investigate the effects of the random fields on the time evolution of the quantum XXZ model in the high-temperature limit. We find that the system with the random fields that satisfy the bimodal distribution undergoes a crossover between a central-peak behavior and a collective-mode one with increasing field when the anisotropy parameter  $\Delta$  is small (e.g.,  $\Delta = 0.01$ ), but the collective-mode behavior vanishes as  $\Delta$  approaches 0.4, then when  $\Delta$  increases to 1.0, the central-peak behavior vanishes and the system just shows a disordered behavior.

The arrangement of this paper is organized as follows. In Sec. 2 we give a simple introduction to the 1-D quantum XXZ model and the recurrence relations method. In Sec. 3 we discuss the results, and Sec. 4 contains a summary.

## 2. MODEL AND METHOD

The Hamiltonian of the 1-D quantum spin-1/2 XXZ model with external fields can be written as

$$H = -\frac{J}{2} \sum_i [(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y) + \Delta \sigma_i^z \sigma_{i+1}^z] - \frac{1}{2} \sum_i B_i \sigma_i^z, \quad (1)$$

where  $\sigma_i^\alpha$  ( $\alpha = x, y, z$ ) are Pauli spin operators,  $J$  and  $\Delta$  are the exchange coupling and the anisotropy parameter, respectively.  $B_i$  denote the external fields, which may be regarded as random variables. Clearly, this Hamiltonian can describe two special cases: the Ising model for which  $\Delta = \infty$  and the isotropy XY model where  $\Delta = 0$ .

The spin autocorrelation function plays an important part in the study of the dynamics of quantum spin systems. It is defined as

$$C(t) = \overline{\langle \sigma_j^x(t) \sigma_j^x(0) \rangle} \quad (2)$$

where  $\overline{\langle \dots \rangle}$  denotes an ensemble average followed by an average over the random variable. The corresponding spectral density which is the Fourier transform of  $C(t)$  can be expressed as

$$\Phi(\omega) = \int_{-\infty}^{+\infty} e^{i\omega t} C(t) dt, \quad (3)$$

and for the mathematical simplicity,  $\Phi(\omega)$  is able to be obtained as

$$\Phi(\omega) = \lim_{\varepsilon \rightarrow 0} \left[ \text{Re} \int_0^\infty dt C(t) e^{-zt} \right], \quad (4)$$

where  $z = \varepsilon + i\omega$ ,  $\varepsilon > 0$ .

The recurrence relations method has been proved to be very powerful in the calculation of dynamic correlation function [13, 23, 24, 27–30, 37]. Next, we will give a brief introduction to this method.

Considering a Hermitian operator  $\sigma_j^x(t)$  as a dynamical variable and then expanding it with an orthogonal set in a Hilbert space,

$$\sigma_j^x(t) = \sum_{\nu=0}^{\infty} a_\nu(t) f_\nu, \quad (5)$$

where  $a_\nu(t)$  are the time-dependent coefficients. There exists the following set of recurrence relation for the basis vectors  $f_\nu$ ,

$$f_{\nu+1} = iL f_\nu + \Delta_\nu f_{\nu-1}, \quad \nu \geq 0, \quad (6)$$

$$\Delta_\nu = \frac{(f_\nu, f_\nu)}{(f_{\nu-1}, f_{\nu-1})}, \quad \nu \geq 1, \quad (7)$$

where  $L \equiv [H, \cdot]$  is the quantum Liouvillian operator,  $(f_\nu, f_\nu) = \overline{\langle f_\nu f_\nu^\dagger \rangle}$ ,  $f_{-1} \equiv 0$  and  $\Delta_0 \equiv 1$ . The coefficients  $a_\nu(t)$  in Eq. (5) satisfy the relation:

$$\Delta_{\nu+1} a_{\nu+1}(t) = -\dot{a}_\nu(t) + a_{\nu-1}(t), \quad \nu \geq 0, \quad (8)$$

where  $\dot{a}_\nu(t) = \frac{da_\nu(z)}{dt}$ ,  $a_{-1}(t) \equiv 0$ .

The spin autocorrelation function  $C(t)$  can be expressed as the form of moment expansion

$$C(t) = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k)!} \mu^{2k} t^{2k}, \quad (9)$$

with

$$\mu^{2k} = \frac{1}{Z} \text{Tr} \sigma_j^x [H, [H, \dots [H, \sigma_j^x] \dots]], \quad (10)$$

where  $\mu^{2k}$  is the  $2k$ th moment of  $C(t)$ . Supposing that the first  $Q$  moments have been calculated by Eq. (10), we can obtain  $C(t)$  by constructing the padé approximate. Because of the mathematical complexity, a finite number of moments can be got, the large times of  $C(t)$  are divergent, thus we just can discuss the short times of  $C(t)$ .

By taking the inner product for  $\sigma_j^x(t)$  and  $\sigma_j^x(0)$ , from Eq. (5), we can find that  $a_0(t)$  is the spin autocorrelation function

$$a_0(t) = \overline{\langle \sigma_j^x(t) \sigma_j^x(0) \rangle} = C(t).$$

Applying the Laplace transform  $a_\nu(z) = \int_0^\infty e^{-zt} a_\nu(t) dt$  ( $z = \varepsilon + i\omega, \varepsilon > 0$ ) to Eq.(8),  $a_0(z)$  in the continued-fraction representation can be obtained as

$$a_0(z) = \frac{1}{z + \frac{\Delta_1}{z + \frac{\Delta_2}{z + \dots}}}. \quad (11)$$

Because we can only get a finite number of recurrants, it is necessary to terminate it with some schemes. Here, we use the Gaussian terminator [13, 38] Which can best serve our problem. With the help of the Padé approximate and the Gaussian terminator, we can obtain the spin autocorrelation function  $C(t)$  and the corresponding spectral density  $\Phi(\omega)$  of the system, respectively.

### 3. RESULTS AND DISCUSSIONS

In order to investigate the spin autocorrelation function  $C(t)$  for  $\sigma_j^x$ , we choose the zeroth basis vector  $f_0 = \sigma_j^x$ . With the recurrence relation Eq. (6), the remaining basis vectors can be obtained:

$$f_1 = B_j \sigma_j^y + J \Delta \sigma_j^y \sigma_{j-1}^z - J \sigma_{j-1}^y \sigma_j^z - J \sigma_{j+1}^y \sigma_j^z + J \Delta \sigma_j^y \sigma_{j+1}^z,$$

$$\begin{aligned} f_2 = & (\Delta_1 - B_j^2 - 2J^2 - 2J^2 \Delta^2) \sigma_j^x + 2J^2 \Delta \sigma_{j-1}^x + 2J^2 \Delta \sigma_{j+1}^x + J^2 \Delta \sigma_{j-1}^x \sigma_{j-2}^y \sigma_j^y \\ & - J^2 \Delta \sigma_{j-2}^x \sigma_{j-1}^y \sigma_j^y + J^2 \sigma_{j+1}^x \sigma_{j-1}^y \sigma_j^y - 2J^2 \sigma_j^x \sigma_{j-1}^y \sigma_{j+1}^y + J^2 \sigma_{j-1}^x \sigma_j^y \sigma_{j+1}^y \\ & - J^2 \Delta \sigma_{j+2}^x \sigma_j^y \sigma_{j+1}^y + J^2 \Delta \sigma_{j+1}^x \sigma_j^y \sigma_{j+2}^y - 2B_j J \Delta \sigma_j^x \sigma_{j-1}^z + (B_{j-1} + B_j) J \sigma_{j-1}^x \sigma_j^z \\ & + (B_{j-1} + B_j) J \sigma_{j+1}^x \sigma_j^z + J^2 \Delta \sigma_{j-1}^x \sigma_j^z \sigma_{j-2}^z - J^2 \sigma_{j-2}^x \sigma_{j-1}^z \sigma_j^z + J^2 \Delta \sigma_{j+1}^x \sigma_j^z \sigma_{j-1}^z \\ & - 2B_j J \Delta \sigma_j^x \sigma_{j+1}^z - 2J^2 \Delta^2 \sigma_j^x \sigma_{j-1}^z \sigma_{j+1}^z + J^2 \Delta \sigma_{j-1}^x \sigma_j^z \sigma_{j+1}^z - J^2 \sigma_{j+2}^x \sigma_j^z \sigma_{j+1}^z \\ & + J^2 \Delta \sigma_{j+1}^x \sigma_j^z \sigma_{j+2}^z, \end{aligned}$$

etc. The first three norms of the basis vectors are obtained as follows:

$$(f_0, f_0) = 1,$$

$$(f_1, f_1) = \overline{B_j^2} + 2\overline{J^2} + 2\overline{J^2\Delta^2},$$

$$(f_2, f_2) = \overline{\Delta_1^2} - 2\overline{\Delta_1 B_j^2} + \overline{B_j^4} - 4\overline{\Delta_1 J^2} + \overline{B_{j-1}^2 J^2} + 2\overline{B_{j-1} B_j J^2} + 6\overline{B_j^2 J^2} + 2\overline{B_{j+1} B_j J^2} \\ + \overline{B_{j+1}^2 J^2} + 12\overline{J^4} - 4\overline{\Delta_1 J^2 \Delta^2} + 12\overline{B_j^2 J^2 \Delta^2} + 24\overline{J^4 \Delta^2} + 8\overline{J^4 \Delta^4}.$$

Then the continued fraction coefficients can be got from Eq. (7).

Next, numerical results of the spin autocorrelation functions  $C(t)$  and the spectral densities  $\Phi(\omega)$  are given when the external fields satisfy three types of distributions: bimodal distribution, Gaussian distribution and double-Gaussian distribution. With special values of the anisotropy parameter  $\Delta$ , the effects of the random external fields on the dynamics of the given system are investigated as follows.

### 3.1. Bimodal distribution

We first consider the case that the external fields satisfy the bimodal distribution.

$$P(B_i) = p\delta(B_i - B_1) + (1 - p)\delta(B_i - B_2). \quad (12)$$

For simplicity and without loss of generality, we choose the exchange coupling  $J = 1.0$ , which sets the energy scale, and the external fields  $B_1 = 1.8$ ,  $B_2 = 0.2$ . For  $\Delta = 0.01, 0.1, 0.4$  and  $1.0$ , the results of the spin autocorrelation function  $C(t)$  and the spectral density  $\Phi(\omega)$  are shown in Fig. 1 and Fig. 2, respectively. The continued-fraction coefficients are presented in the insets.

When  $\Delta$  is small (e.g.,  $\Delta = 0.01, 0.1$ ), the spin autocorrelation function [see in Figs. 1(a1), (a2)], changes from a monotonically decreasing behavior to a damped oscillatory one as  $p$  increases. When  $p = 0$ , the exchange coupling energy is higher than the external field energy. The interaction among the spins is stronger than that between the spin and the external field. The dynamics is dominated by the exchange coupling energy and shows a central-peak behavior. When  $p = 0.25$ , the spin autocorrelation function has a slight fluctuation and the fluctuation becomes acute with the increase of the external fields. When  $p = 1$ , the value of the external field is larger than that of the exchange coupling. The system behaves as the precession of independent spins about the field and the exchange coupling causes a damping. Hence, the system presents a collective-mode behavior. Figs. 2(b1) and (b2) show that the peak of  $\Phi(\omega)$  moves from  $\omega = 0$  to  $2$  as  $p$  increases, which also

reaches the conclusion that the system undergoes a crossover from the central-peak behavior to the collective-mode one with increasing field when  $\Delta$  is small.

Figure 1(a3) shows that when  $\Delta = 0.4$ , the dynamics of the system changes from a central-peak regime to a disordered behavior which is intervenient between a central-peak one and a collective-mode one as  $p$  increases. The spin autocorrelation function for  $p = 0$  decays monotonically to 0 and the spectral density is now peaked at  $\omega = 0$ . So, the system is at the central-peak regime where the dynamics is mostly dominated by the exchange coupling. By comparing the curve for  $p = 0$  in Figs. 1(a1) or (a2) to the one in Fig. 1(a3), we find that  $C(t)$  for  $\Delta = 0.4$  decays faster than that for  $\Delta = 0.01$  or  $\Delta = 0.1$ . As  $p$  increases to 1.0, the system shows not a collective-mode behavior but a disordered one. The spectral density displayed in Fig. 2(b3) tends to have an expansion at high frequency.

When  $\Delta = 1.0$  [see Figs. 1(a4) and 2(b4)], the system presents a disordered behavior as the concentration of  $B_1$  increases, i.e., in this case, the dynamics of the system can not be characterized by either behavior singly. Specially the case of  $p = 0$  is very similar to the most-disordered case mentioned in Ref. [23]. By comparing the results when  $\Delta = 0.01$  to that of the 1-D XY model, we find that they are very similar, so the effect of the anisotropy parameter can be basically ignored, in other words, the dynamics of the system is governed by the competition between spin-spin interactions and the external fields. Comparing Figs. 1(a1), (a2), (a3) and (a4), it can be found that as the anisotropy parameter  $\Delta$  increases, the crossover from the central-peak behavior to the collective-mode one vanishes. When  $\Delta = 1.0$ , the system becomes the 1-D quantum Heisenberg system. The anisotropy parameter together with the external field and the exchange coupling decide the dynamic behaviors of the system. The competition between the spin-spin interactions and the external fields becomes very fierce which drives the system to be disordered.

### 3.2. Gaussian distribution

In the case, the external fields satisfy the Gaussian distribution,

$$P(B_i) = \frac{1}{\sqrt{2\pi}\sigma_B} \exp \left[ - (B_i - B)^2 / 2\sigma_B^2 \right], \quad (13)$$

where  $B$  is the mean value of the external fields,  $\sigma_B$  is the standard deviation. Here, we take the exchange coupling  $J$  equal to 1.0 and  $B$  equal to 0.0, 0.5, 1.0, 1.5, 2.0. When the

anisotropy parameter  $\Delta = 0.1, 0.4$  and  $1.0$ , the results of the spin autocorrelation function and the spectral density are displayed in Fig. 3 for  $\sigma_B = 0.3$  and Fig. 4 for  $\sigma_B = 3.0$ .

Figure 3(a1) shows that when the standard deviation is small ( $\sigma_B = 0.3$ ) and  $\Delta = 0.1$ , the system shows two types of dynamics as  $B$  increases: the central-peak behavior and the collective-mode behavior. In this case, the effect of  $\Delta$  can be ignored basically, the dynamics of the system changes according to the concentration of  $B$ . As  $\Delta$  increases from  $0.1$  to  $1.0$ , a disordered behavior replaces the central-peak behavior or the collective-mode behavior. Figs. 3(a2), (b2) and (c2) also show that the effects of the external fields are to urge the system to show a crossover when  $\Delta = 0.1$  and as  $\Delta$  increases to  $1.0$ , the system displays a disordered behavior.

When the standard deviation is large enough ( $\sigma_B = 3.0$ )[see Fig. 4], the system just shows a disordered behavior which is something in between the central-peak behavior and the collective-mode one regardless of the anisotropy parameter. From Fig. 3 and Fig. 4, it is not difficult to see that both the crossover and disordered behavior are replaced by one disordered behavior with the increase of  $\sigma_B$ . This is because the value of the external field is large and the value range is wide when  $\sigma_B = 3.0$ . The large external fields drive the spin orientation of the system to be disordered.

### 3.3. Double-Gaussian distribution

Double-Gaussian distribution is a common form of bimodal distribution and Gaussian distribution, which can be used to describe both discrete distribution and continuous one,

$$P(B_i) = p \frac{1}{\sqrt{2\pi}\sigma_B} \exp \left[ -(B_i - B_1)^2 / 2\sigma_B^2 \right] + (1 - p) \frac{1}{\sqrt{2\pi}\sigma_B} \exp \left[ -(B_i - B_2)^2 / 2\sigma_B^2 \right], \quad (14)$$

where  $0 \leq p \leq 1$  represents the concentration of  $B_1$  that satisfies the Gaussian distribution. The external fields satisfy Eq. (14), in which the mean values  $B_1 = 1.8$  and  $B_2 = 0.2$ , and the exchange coupling is constant ( $J = 1.0$ ).  $C(t)$  and  $\Phi(\omega)$  for  $\Delta = 0.1, 0.4$  and  $1.0$  are calculated and the results are shown in Fig. 5 and Fig. 6, respectively. The figures indicate that when  $\sigma_B = 0.3$ , the system for  $\Delta = 0.1$  shows a crossover between a central-peak behavior and a collective-mode one, and a disordered behavior as  $\Delta$  increases to  $1.0$ . However, the system only shows a disordered behavior when  $\sigma_B = 3.0$ , no matter what  $\Delta$  takes.



From above discussion, we can see that the dynamical behavior of the system is affected by the competition between the spin-spin interactions and the external fields, not by the different disordered distribution. Also, it is easy to find that the dynamics of the system is similar to that of the 1-D quantum XY model [28] when  $\Delta$  is small (e.g.,  $\Delta = 0.01$ ). When  $\Delta = 0$ , the XXZ model becomes the isotropy XY model. We find that the above results are the same as those in Ref. [28] when we take  $\Delta = 0$ .

#### 4. SUMMARY

We have studied the dynamics of the 1-D spin-1/2 quantum XXZ model in the random external fields at the high-temperature limit by means of the recurrence relations method. We find that the dynamics of the system with three types of random distributions are affected by the competition among the external field, the anisotropy parameter and the exchange coupling, but the anisotropy parameter can be basically ignored when it is small (e.g.,  $\Delta = 0.01$ ). For the case of bimodal disorder, when the anisotropy parameter  $\Delta$  is small (e.g.,  $\Delta = 0.01$ ), the dynamics of the system undergoes a crossover between a collective-mode behavior and a central-peak one with increasing field; as  $\Delta$  increases to 0.4, the dynamics of the system changes from a central-peak regime to a disordered behavior which is intervenient between a central-peak one and a collective-mode one with the increase of the fields; then as  $\Delta$  approaches 1, the system shows a disordered behavior. In the cases of Gaussian disorder and double-Gaussian disorder, when the standard deviation of the random field  $\sigma_B$  is small, a disordered behavior replaces the crossover as  $\Delta$  increases. When  $\sigma_B$  becomes large enough, the system shows only a most disordered behavior regardless of the anisotropy parameter.

#### Acknowledgments

This work was supported by the National Natural Science foundation of China under Grant NO. 10775088, the Shandong Natural Science foundation under Grant NO. Y2006A05, and the Science foundation of Qufu Normal University. One of the authors (Yin-Yang Shen)

thanks Shu-Xia Chen, Fu-Wu Ma, Hong Li and Sha-Sha Li for useful discussions.

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## Figure Captions

Fig. 1 The spin autocorrelation functions where the external fields take the values  $B_1 = 1.8$  with probability  $p$  and  $B_2 = 0.2$  with probability  $(1 - p)$ . (a1), (a2), (a3), (a4) correspond to the cases of  $\Delta = 0.01, 0.1, 0.4$  and  $1.0$ . The continued-fraction coefficients are presented in the insets.

Fig. 2 The corresponding spectral densities for the same parameters as in Fig. 1. (b1), (b2), (b3), (b4) correspond to the cases of  $\Delta = 0.01, 0.1, 0.4$  and  $1.0$ .

Fig. 3 The spin autocorrelation functions and the spectral densities for the case that the external fields satisfy the Gaussian distribution. The standard deviation  $\sigma_B$  takes  $0.3$ . (a1), (a2) correspond to the case that  $\Delta$  equals to  $0.1$ , (b1), (b2) correspond to the case that  $\Delta$  equals to  $0.4$ , and (c1), (c2) correspond to the case that  $\Delta$  equals to  $1.0$ .

Fig. 4 The spin autocorrelation functions and the spectral densities for the case that the external fields satisfy the Gaussian distribution. The standard deviation  $\sigma_B$  takes  $3.0$ . (a1), (a2) correspond to the case that  $\Delta$  equals to  $0.1$ , (b1), (b2) correspond to the case that  $\Delta$  equals to  $0.4$ , and (c1), (c2) correspond to the case that  $\Delta$  equals to  $1.0$ .

Fig. 5 The spin autocorrelation functions for the case that the external fields satisfy the double-Gaussian distribution in which the mean values  $B_1 = 1.8$  and  $B_2 = 0.2$  with probabilities  $p$  and  $(1 - p)$ . (a1), (a2) and (a3) correspond to the case that the standard deviation  $\sigma_B$  takes  $0.3$  and  $\Delta$  takes the value  $0.1, 0.4, 1.0$ , respectively. (b1), (b2) and (b3) correspond to the case that the standard deviation  $\sigma_B$  takes  $3.0$  and  $\Delta$  takes the value  $0.1, 0.4, 1.0$ , respectively.

Fig. 6 The spectral densities for the same parameters as in Fig. 5. (a1), (a2) and (a3) correspond to the case that the standard deviation  $\sigma_B$  takes  $0.3$  and  $\Delta$  takes the value  $0.1, 0.4, 1.0$ , respectively. (b1), (b2) and (b3) correspond to the case that the standard deviation  $\sigma_B$  takes  $3.0$  and  $\Delta$  takes the value  $0.1, 0.4, 1.0$ , respectively.













